

The Impacts of Biogenic Emissions Estimates from BEIS-3 on Ozone Modeling in the Southeastern US

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ABSTRACT

Biogenic emissions are a significant component of the total emissions that contribute to the formation of ozone in the Southeastern US. Photochemical air quality simulation models, used for studying air quality problems for research as well as regulatory applications, use emissions processing systems to prepare inputs to the modeling systems. A new prototype of the emissions processor to prepare model-ready biogenic inputs, namely, the Biogenic Emissions Inventory System (BEIS-3 Vers.1) has recently been developed. BEIS-3 is compatible with the Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system and uses the Input/Output Applications Programming Interface (I/O API) format. For this study, an implementation of BEIS-3 in SMOKE has been used to prepare the biogenic emissions inputs, and a sensitivity simulation performed using the Multiscale Air Quality Simulation Platform (MAQSIP) application for the June 19-30, 1996 episode in North Carolina. This period was characterized by high ozone in the Charlotte-Gastonia-Rock Hill, Greensboro-Winston Salem-High Point, and Raleigh-Durham-Chapel Hill areas. Horizontally, MAQSIP employs a nested 36/12/4-km grid resolution for this application, with the 4-km grid covering almost the entire state of NC. In using the BEIS-3 emissions estimates for MAQSIP, it was found that significant amounts of emissions of alcohols (MEOH and ETOH) were estimated from BEIS-3, that were not explicitly treated by the Carbon Bond (CB4) chemical mechanism. We then updated the chemical mechanism used in MAQSIP to include explicit treatment of these two alcohol species. To assess the complete effects of the additional alcohol species in the modeling system, we present analyses of the model predictions of several other species related to the biogenic methanol and ethanol oxidation reactions. The impact of using an updated biogenic emissions processor on model performance for ozone in a regulatory setting, and ongoing work, are discussed.

INTRODUCTION

Emissions of nitrogen oxides and volatile organic compounds (VOCs) from anthropogenic and biogenic sources react in the presence of sunlight to form ozone in the atmosphere. Motivated by health effect concerns of ozone and its precursors, the Clean Air Act Amendments of 1990 established selected comprehensive, three-dimensional (3-D) photochemical air quality simulation models (PAQSMs) as the required regulatory tools for analyzing the urban and regional problem of high ambient ozone levels across the United States. These models are currently applied to study and establish strategies for meeting the National Ambient Air Quality Standard (NAAQS) for ozone nonattainment areas¹. State Implementation Plans (SIPs) resulting from these efforts must be submitted to the U.S. Environmental Protection Agency (EPA). The use of grid-based photochemical models has expanded dramatically during the past decade to include spatial scales varying from urban to regional. Despite significant progress in photochemical modeling science in the last decade, large uncertainties still remain on the role of biogenic emissions in the formation of ozone. While it is extremely difficult to quantify the uncertainty levels of biogenic emissions estimates due to lack of data, a factor of three is probably a reasonable estimate for total VOCs nationwide²; but predictions for specific regions and periods could vary even more. It is critical that this area be studied extensively since the contribution of emissions

from natural sources has significant implications towards the choice and extent of controls needed on anthropogenic sources in order to attain NAAQS in a given region.

Biogenic emissions are released from a variety of ecosystems ranging from forests to grasslands, and even urban landscapes. These biogenic emissions consist of a variety of VOCs emitted from vegetation (e.g., isoprene, monoterpenes, sesquiterpenes, and oxygenated VOCs like methyl butenol, methanol, acetaldehyde, etc.), inorganic compounds emitted from soils (NO), and vegetation (CO). On a global scale, natural emissions of these species equal or exceed anthropogenic sources. While the magnitude of biogenic and anthropogenic VOC emissions are approximately comparable on a nation-wide basis³, their relative magnitudes somewhat vary on a urban-to-regional basis, and hence need to be properly estimated for use in regional-scale air quality modeling systems. These biogenic emissions have typically been estimated using the Biogenic Emissions Inventory Systems (BEIS)^{4,5,6,7} to prepare air quality model ready emissions inputs. Models like BEIS are used to estimate emissions from various biogenic sources, chemically speciate, temporally and spatially allocate to the resolution of the modeling system being used.

Until most recently, two generations of BEIS models have been used to provide emissions estimates from natural sources for use in air quality models. BEIS-3⁷ is the new third-generation model, which uses the most recent science that has been made available.

OBJECTIVE

The objective of this study is to evaluate the impacts of using biogenic emissions estimates from the new BEIS-3/SMOKE modeling system on ozone predictions in the Southeastern United States. Specifically, we generated biogenic emissions estimates from BEIS-2 and BEIS-3 and performed MAQSIP simulations over a nested configuration of 36/12/-4 km grids centered over North Carolina for the June 19-30, 1996 episode, and compared model predictions from the two scenarios, and comment on the comparative use of these systems in regulatory applications toward attainment of the NAAQS for ozone.

EPISODE DESCRIPTION

The period we simulated was June 19-30, 1996. This is one of the episodes that has been chosen to support modeling for the 8-h ozone attainment demonstration in North Carolina (NC)⁸. This actually consists of two separate episodes, from June 21-24, and June 27-30. They were modeled and evaluated at the same time, so the statistics and episode composite evaluation cover all days of the two episodes. Some of the analyses however are presented only for the eight episode days.

MODELING SYSTEMS

The modeling domain used for this study has a nested system of 36-, 12-, and 4-km grids centered over NC (Figure 1). The descriptions of the various models used are given below:

Mesoscale Model (MM5)

The meteorological inputs for this study were derived from the Fifth-Generation Penn State/NCAR Mesoscale Model Version 2 (MM5 V2.12)⁹. The configuration of the MM5 modeling system is given in Table 1.

Table 1. MM5 model configuration.

Grid	Col, Row	Cloud Treatment	Model Time step	PBL Scheme
108 -km	54 X 42	Kuo	300 s	Gayno-Seaman
36-km	60 X 60	Kain-Fritsch	100 s	Blackadar
12-km	81 X 63	Kain-Fritsch	36 s	Blackadar
4-km	126 X 75	None (Explicit)	12 s	Blackadar

An iterative procedure was used to generate the best meteorological inputs possible. The meteorological model performance was evaluated each time to measure improvements. The model contains two types of planetary boundary layer (PBL) parameterizations suitable for air quality modeling applications, both of which represent subgrid-scale fluxes of heat, moisture, and momentum. A modified Blackadar PBL scheme uses a first-order eddy diffusivity formulation suitable for stable and neutral environments and a nonlocal closure for unstable regimes. The Gayno-Seaman PBL scheme uses a prognostic equation for the second-order turbulent kinetic energy, while diagnosing the other key boundary layer terms.

MM5 was vertically resolved into 26 layers, and the top of the domain extended up to 16 km. While the first layer had a height of 38 m, there were 9 layers within the lowest 1 km. No interpolations are necessary from MM5 to MAQSIP in the horizontal or vertical since the models all use the same coordinate systems and grid configurations. To generate MAQSIP-ready inputs, MM5 was executed in the coupled mode along with MCPL¹⁰; MCPL is a drop-in MM5 output module designed for coupling MM5 to other environmental models, using the EDSS/Models-3 I/O API. It fits into MM5 as a subroutine that is called every output time step by the MM5v2 driver or from the SOLVE routine.

Multiscale Air Quality Simulation Platform (MAQSIP)

MAQSIP is a comprehensive urban to intercontinental scale atmospheric chemistry-transport model, developed at the MCNC–Environmental Modeling Center in collaboration with EPA; the model also served as a prototype for EPA’s CMAQ modeling system^{11, 12}. In its current form, MAQSIP has been used at various scales to study problems related to tropospheric ozone, acidic substances, and aerosol formation and pollutant distribution for a variety of geographic areas of the world. MAQSIP has been applied to simulate tropospheric ozone distributions and trends over the eastern United States on a seasonal scale for 1995 and model predictions have been rigorously evaluated against available observations from surface and aircraft measurements from the Southern Oxidant Study databases^{13, 14, 15}. On the regulatory side, MAQSIP is currently being applied in the states of North Carolina⁸ and Virginia. Recently, MCNC adapted the MAQSIP/MM5/SMOKE system to produce operational real-time forecasts for ozone over the eastern United States.¹⁶

While MAQSIP can emulate many existing atmospheric chemistry-transport models, its modular and flexible structure facilitates incorporation of new, improved process representations and algorithms. This capability allows the system to be used as a comprehensive test-bed environment for exploring different process and algorithmic representations in situ in a 3-D modeling framework with other interacting physical and chemical phenomena. Its modularity also facilitates adapting the model to address a broad range of atmospheric chemistry and transport problems. MAQSIP is formulated with a generalized coordinate system^{17, 18} to better interface the chemistry-transport calculations with various meteorological models. MAQSIP’s formulation supports multiple nesting of grids for efficient resolution of smaller-scale phenomena, and allows for full interaction between disparate spatial scales. Thus, the model can be adapted to a variety of spatial domains ranging from urban to interregional with flexible grid resolution; simulations to date have used 4-km to 100-km grid resolutions. The model also

has the flexibility to use different chemical mechanisms for representing gas-phase chemistry or for incorporating explicit chemical schemes. Since the Carbon Bond (CB4) chemical mechanism¹⁹ has been the most widely used chemical mechanism for most regulatory applications, we used the CB4 mechanism here. The effects of cloud transport on the vertical distribution of trace species in the atmosphere are represented either with the Kain-Fritsch or the Kuo-Anthes scheme, depending on the scale of model application and on the scheme used in the input meteorological driver.

Sparse Matrix Operator Kernel Emissions (SMOKE)

Emissions inputs to the model were developed using the Sparse Matrix Operator Kernel Emissions (SMOKE)¹⁸ processing system. Biogenic emissions were processed using an implementation of BEIS-2 and the newly implemented²¹ BEIS-3 within SMOKE.

Biogenic Emissions Inventory System (BEIS-3)

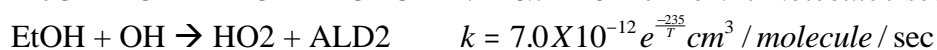
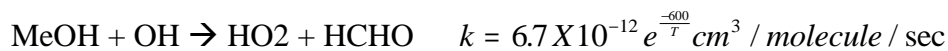
Details of the implementation of BEIS-3 within SMOKE²¹ are available separately. Key features of BEIS-3 are listed below:

- 1-km resolution landuse data obtained from the Biogenic emissions landcover (BELD3v3.1) database²²
- 230 different landuse types
- Extensive list of emitted compounds, i.e. normalized emissions for 34 different species, including 14 monoterpenes
 - 34 BEIS-3 species, subsequently mapped to 12 species in the CB4 chemical mechanism (CO, NO, ALD2, ETH, ETOH, FORM, ISOP, MEOH, OLE, PAR, TOL, and XYL)
 - BEIS-2 had only five CB4 species (NO, ALD2, ISOP, OLE, PAR)
- Treats natural emissions of NO from soils, biomass burning, and lightning
- Treats CO production from soils and biomass burning
- Campbell and Norman light correction factor for isoprene and methyl butenol (MBO)
- Uses surface pressure information, in addition to temperature and radiation data

BEIS-3 in MAQSIP

We evaluated the impact of biogenic estimates from BEIS-3 in MAQSIP in a phased manner. In the first two rounds, we performed sensitivity modeling only in the 4-km modeling domain. In the first round, MAQSIP was simulated without any changes in the chemistry, and we saw increases in mean layer one 1-h O₃ by a fraction of a ppb. In the second round, MEOH and ETOH emissions were treated as paraffins as a first approximation. A conversion factor of MEOH = PAR, and ETOH = 2PAR was used and the alcohols were treated as paraffins in the MAQSIP chemistry. This sensitivity also yielded a fractional increase by a ppb in both mean 1-h and 8-h O₃ across the 4-km modeling domain.

Finally in the third round, to explicitly treat the MEOH and ETOH species, the MAQSIP CB4 chemistry was updated to include the following two reactions involving alcohol oxidation. The rate constants for these reactions were obtained from literature²³.



The dry deposition velocities for paraffins (PAR) were used as the approximate dry deposition velocities for the two alcohol species. The biogenic emissions were now estimated for all the 36/12/4-

km grids and MAQSIP was rerun with explicit chemistry. The results of this simulation will be presented in detail, in the next section, along with comparisons from earlier simulations with BEIS-2 emissions estimates.

MODEL PERFORMANCE EVALUATION

EPA has developed guidance documents^{1, 24} for photochemical model performance evaluation that suggest specific tests and comparisons, recommend graphical methods for use in interpreting and displaying results, and identify potential issues or problems that may arise. Besides using these recommendations, we also included a comprehensive set of additional statistics in a technical report prepared for the California Air Resources Board²⁵ in the evaluation of the model performance. Concentration cut-off thresholds at 40 ppb or 60 ppb have historically been used in computing the statistical measures in model performance evaluation studies in urban settings. However, using thresholds results in significant information loss relative to the models' ability to capture the full diurnal cycle in ozone and NO_x, with the result that the final interpretation of model behavior is potentially distorted²⁶. While some model underpredictions (observed concentration above the cutoff and modeled concentrations below it) are included in the estimate, some overpredictions (observed concentration below and modeled concentration above the cutoff) are excluded. Thus, we computed the various statistical measures for the subday divisions without using any threshold. In line with the regulatory settings, the statistical measures for all 24 hours in each day (without any subday divisions) were computed at a threshold of 40 and 60 ppb as well as at 5 ppb (essentially using the entire dataset).

ANALYSES

Figures 2 and 3 illustrate the differences in domain-wide emissions estimated from BEIS-2 and BEIS-3 for the 36, 12, and 4-km modeling domains. While Figure 2 shows the comparisons by way of bar charts for biogenic emissions alone, the pie charts in Figure 3 compare the total VOCs (from both anthropogenic and biogenic sources). The additional biogenic species from BEIS-3 and their magnitudes are seen in Figure 2. In Figure 3, since the anthropogenic emissions estimates remained the same in the two cases, the differences are solely from BEIS-3's biogenic estimates. The sizes of the pie for BEIS-3 in each grid are scaled relative to the total VOCs in BEIS-2. From the total emissions listed under each pie, it is seen that total VOCs in the BEIS-3 case increased by 58%, 52% and 40% compared to BEIS-2 in the 36, 12 and 4-km grids respectively. The substantial differences in biogenic emissions estimates compared to BEIS-2 were partially due to the new landcover data. Improved landcover/biomass distribution data resulted in significant changes in the emissions inventory. While the percent of isoprene in total VOCs (from anthropogenic and biogenic sources) went down from BEIS-2 to BEIS-3, the magnitude of isoprene emissions actually went up by 17%, 18% and 4% in the 36, 12 and 4-km grids respectively. Other than isoprene, large increases are seen in MEOH, ETOH and FORM. With the use of BEIS-3, ALD2, PAR, and NO emissions from biogenic sources decreased (NO not shown on these plots). On a domain-wide basis, the decrease in total NO budget (from anthropogenic and biogenic sources) ranged from 1-3% in the three grids.

Isoprene has been extensively studied, and regional emissions inventories of isoprene have been developed with reasonable accuracy in the past. However the estimates for the newer biogenic VOCs modeled with BEIS-3, (oxygenated VOCs like MEOH and ETOH) have not been verified so far. To obtain more confidence in modeling these species explicitly in air quality models, we need to corroborate emissions estimates of these species with ambient measurements.

We performed evaluation of the model performance for 1-h O_3 in all the three modeling grids, and used observed data from EPA's Aerometric Information Retrieval System (AIRS). Various measures of performance were computed at observed thresholds of 5, 40 and 60 ppb, and shown in Table 2. Figure 4 shows the observed mean 1-h O_3 at all sites in each of the domain compared to the predicted mean 1-h O_3 from the two modeling simulations with BEIS-2 and BEIS-3. Overall, these measures show that the predictions from BEIS-3 are higher than those with BEIS-2 by 2-3 ppb. The differences are higher as the observed threshold concentration increases from 5 to 60 ppb. While this positive bias in BEIS-3 versus BEIS-2 somewhat lowers the model performance measures at 5 ppb threshold, the model performance measures at 60 ppb are better with BEIS-3.

The predicted daily maximum 8-h O_3 concentrations from MAQSIP simulations using BEIS2 and BEIS-3 in the NC portion of the 4-km grid are used to generate Air Quality Index (AQI) counts of the number of grid-cells in NC falling within each of the 4 AQI bins recommended by EPA²⁷. We generated these counts for each episode-day as well as for the entire episode, and plotted them as stacked bar charts shown in Figure 5. On all the days, while the Code Green and Code Yellow counts decrease in BEIS-3, there is an increase in Code Orange and Code Red.

To obtain an estimate of how the change in biogenic emissions estimates might impact the accuracy of peak predictions (paired in space and time), the predicted daily maximum 1-h and 8-h O_3 concentrations from BEIS-2 and BEIS-3 at all grid-cells containing ozone monitors are shown as scatter-plots for the 12 and 4-km grids in Figures 6a-6d. In these plots, we disaggregated the data points into three groups, namely Rural, Suburban and Urban (based upon AIRS classification for ozone monitors) to see if there was a bias in model performance based upon its location. A 1:1 line is also added for reference purposes on these plots. For all the cases, the daily maxima from BEIS-3 are higher than BEIS-2. Thus, while BEIS-3 shows an overall positive bias compared to BEIS-2, no consistent bias was seen in these predictions, based upon the monitor location type.

An understanding of the complete effects of the BEIS-3 estimates on these two simulations can be obtained by comparing predictions of model species other than ozone. We undertook some preliminary comparisons here for species associated with the alcohol oxidation processes. The addition of larger amounts of MEOH and ETOH emissions along with their explicit chemical treatment led to large amounts of radical sources. Alcohol oxidation is a source of radicals - both directly, with the production of hydroperoxy radicals, and indirectly, with the production of lower and higher aldehydes (formaldehyde [FORM] and RCHO). Both these aldehydes rapidly decompose to other radicals and radical precursors like peroxyacetyl nitrate (PAN). Overall, it is this positive change in the radical budget that led to increased ozone formation from BEIS-3. Using integrated process analyses/integrated reaction rate analyses (IPR/IRR) might provide additional insight into the model predictions from a model process perspective. We plan to undertake these tasks in continuing evaluation of BEIS-3 in MAQSIP.

Figure 1. MAQSIP modeling domain showing the 36-, 12- and 4-km grids.

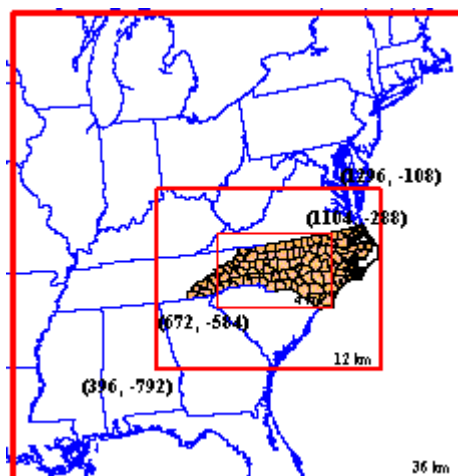


Table 2. Model performance measures for 1-h O₃ computed for the entire episode (June 19-30, 1996).

CASE	Grid	ObsThr (ppb)	# pairs	ModAvg (ppb)	ObAvg (ppb)	Bias (ppb)	Error (ppb)	R ²	Nbias	Gerror
BEIS2	4km	5	10857	57.5	49.6	7.9	16.5	0.398	-0.460	0.607
BEIS3			10857	59.2	49.6	9.6	17.2	0.396	-0.501	0.634
BEIS2	12km	5	24335	55.4	47.9	7.5	17.1	0.348	-0.525	0.700
BEIS3			24335	57.3	47.9	9.5	18.0	0.350	-0.577	0.732
BEIS2	36km	5	43328	53.2	46.5	6.8	17.2	0.332	-0.483	0.683
BEIS3			43328	55.6	46.5	9.2	17.8	0.346	-0.549	0.714
BEIS2	4km	40	6715	65.6	64.9	0.7	12.7	0.246	-0.041	0.211
BEIS3			6715	67.4	64.9	2.6	13.3	0.243	-0.070	0.223
BEIS2	12km	40	14617	63.6	63.8	-0.3	13.4	0.246	-0.020	0.224
BEIS3			14617	65.8	63.8	2.0	14.1	0.244	-0.056	0.236
BEIS2	36km	40	25049	62.0	62.7	-0.7	14.4	0.218	-0.010	0.244
BEIS3			25049	64.8	62.7	2.1	14.5	0.228	-0.056	0.249
BEIS2	4km	60	3684	71.7	76.4	-4.7	11.7	0.149	0.050	0.152
BEIS3			3684	73.7	76.4	-2.8	11.8	0.151	0.025	0.154
BEIS2	12km	60	7733	70.6	75.6	-5.0	13.0	0.157	0.057	0.171
BEIS3			7733	73.0	75.6	-2.5	13.2	0.156	0.024	0.176
BEIS2	36km	60	12639	69.6	74.8	-5.2	13.7	0.128	0.061	0.184
BEIS3			12639	72.7	74.8	-2.1	13.3	0.139	0.020	0.181

Figure 2. Total VOCs from biogenic sources in the modeling domain on June 24, 1996.

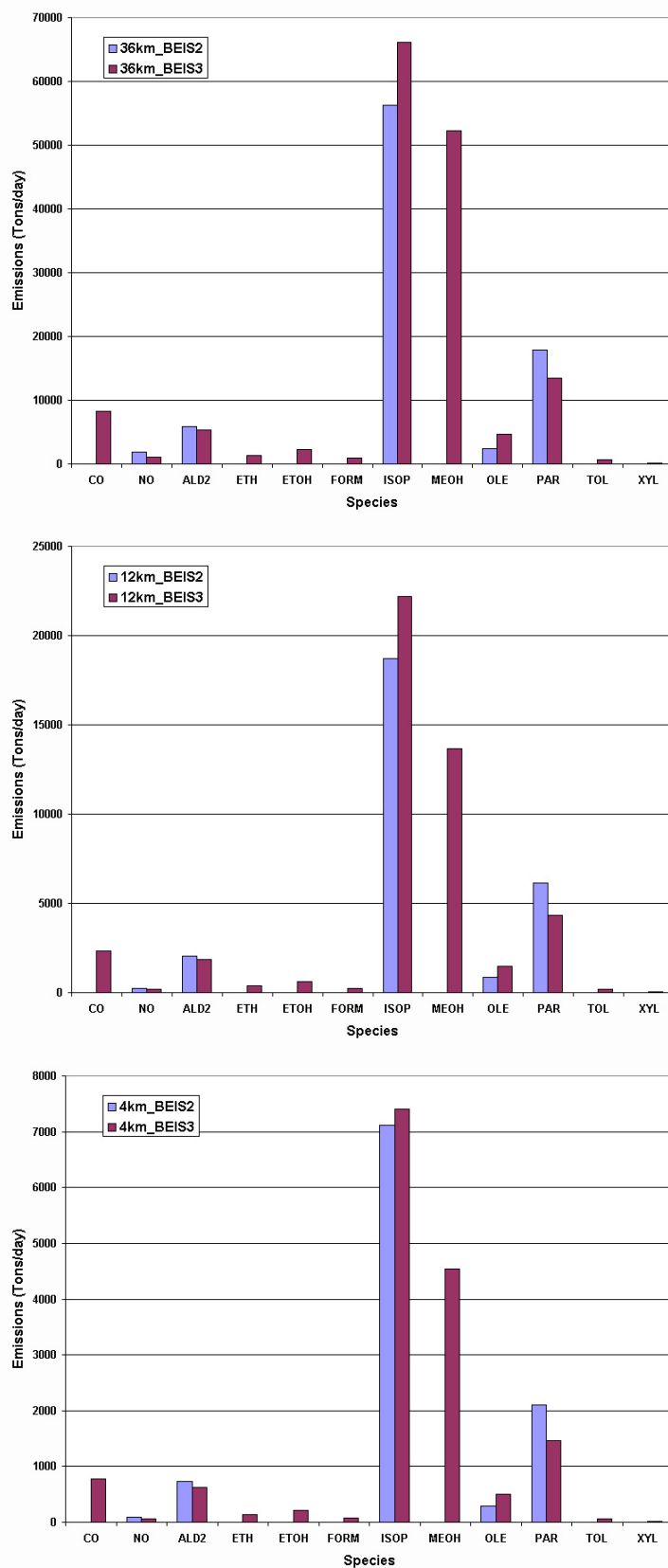


Figure 3. Total anthropogenic and biogenic VOCs in the modeling domain on June 24, 1996.

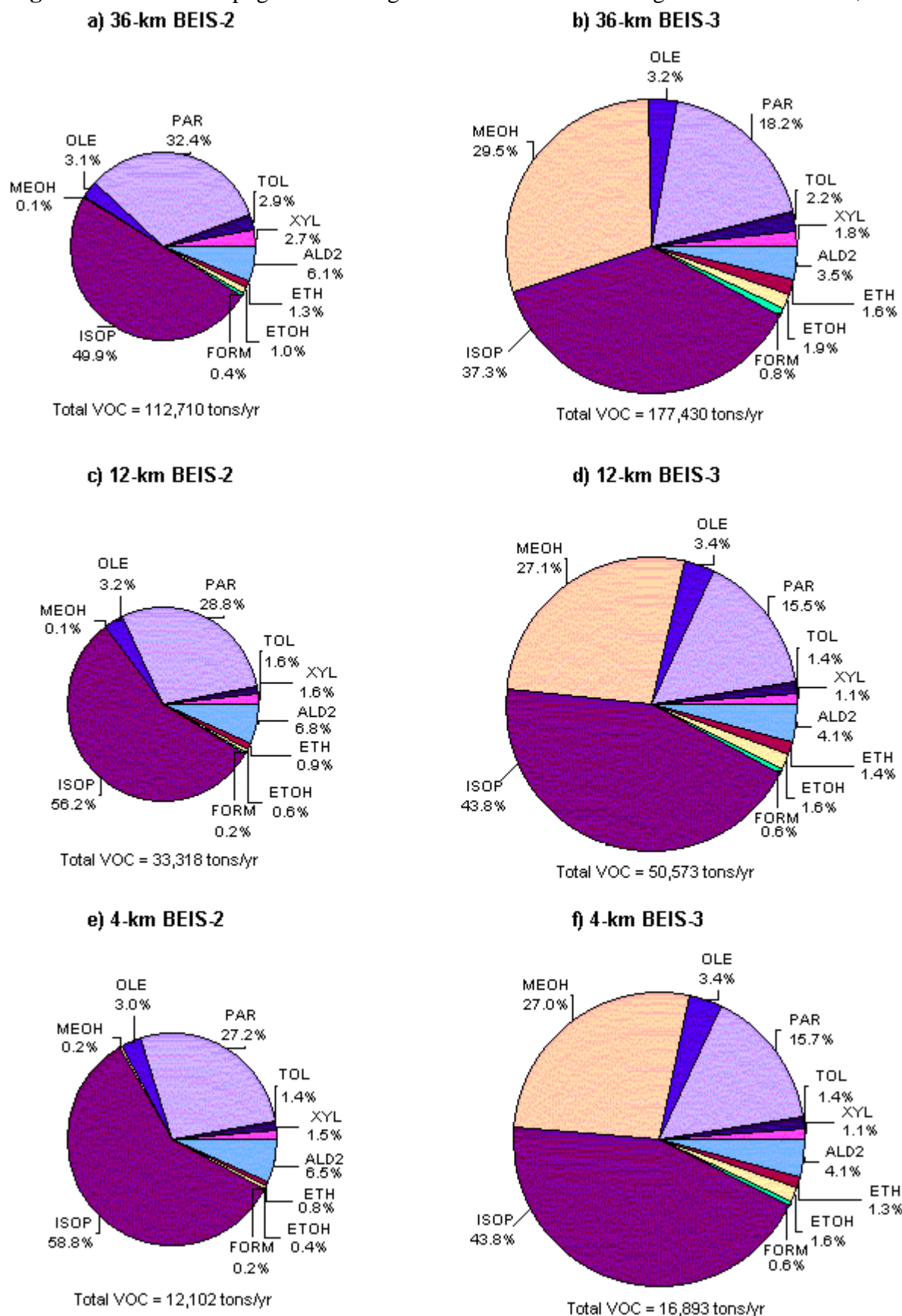
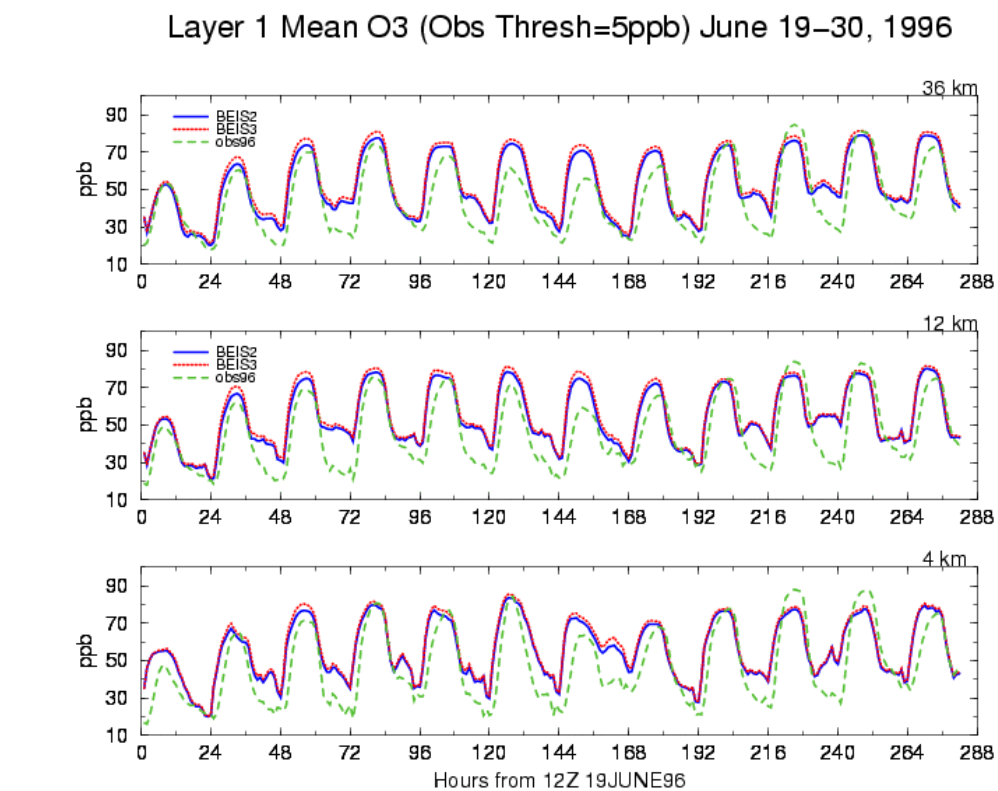
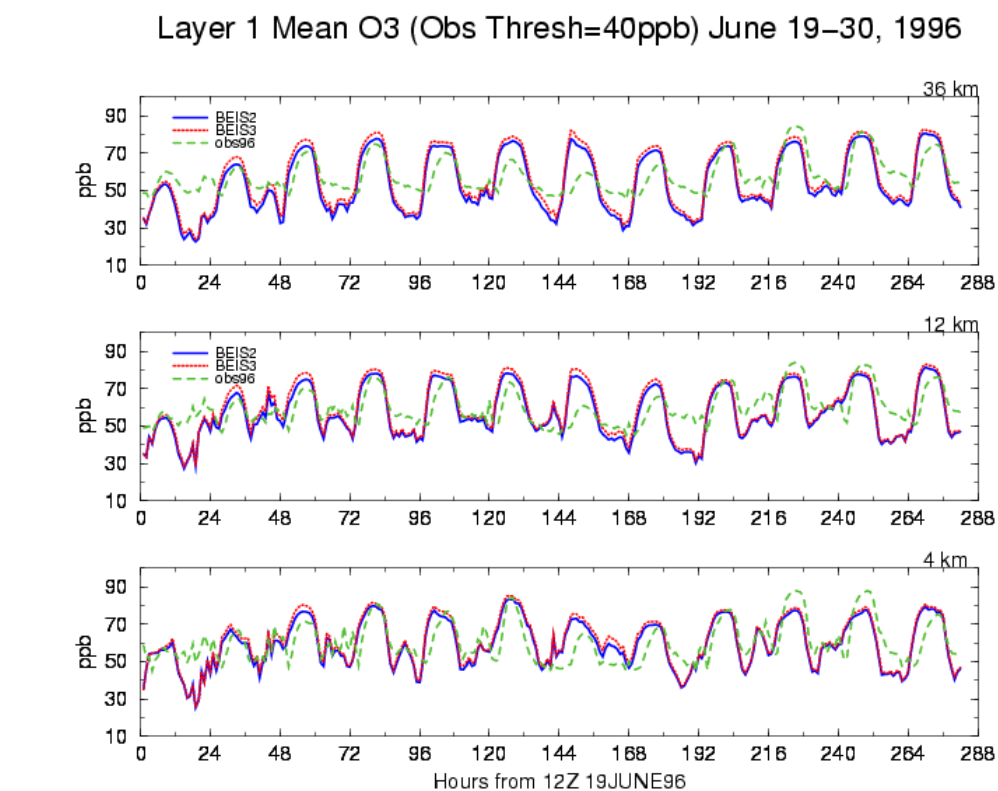


Figure 4. Mean 1-h O_3 concentrations with observed thresholds of 5 ppb (top) and 40 ppb (bottom).



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Figure 5. Air Quality Index (AQI) based grid-cell counts in the 4-km NC mask for MAQSIP simulations with BEIS-2 (top) and BEIS-3 (bottom).

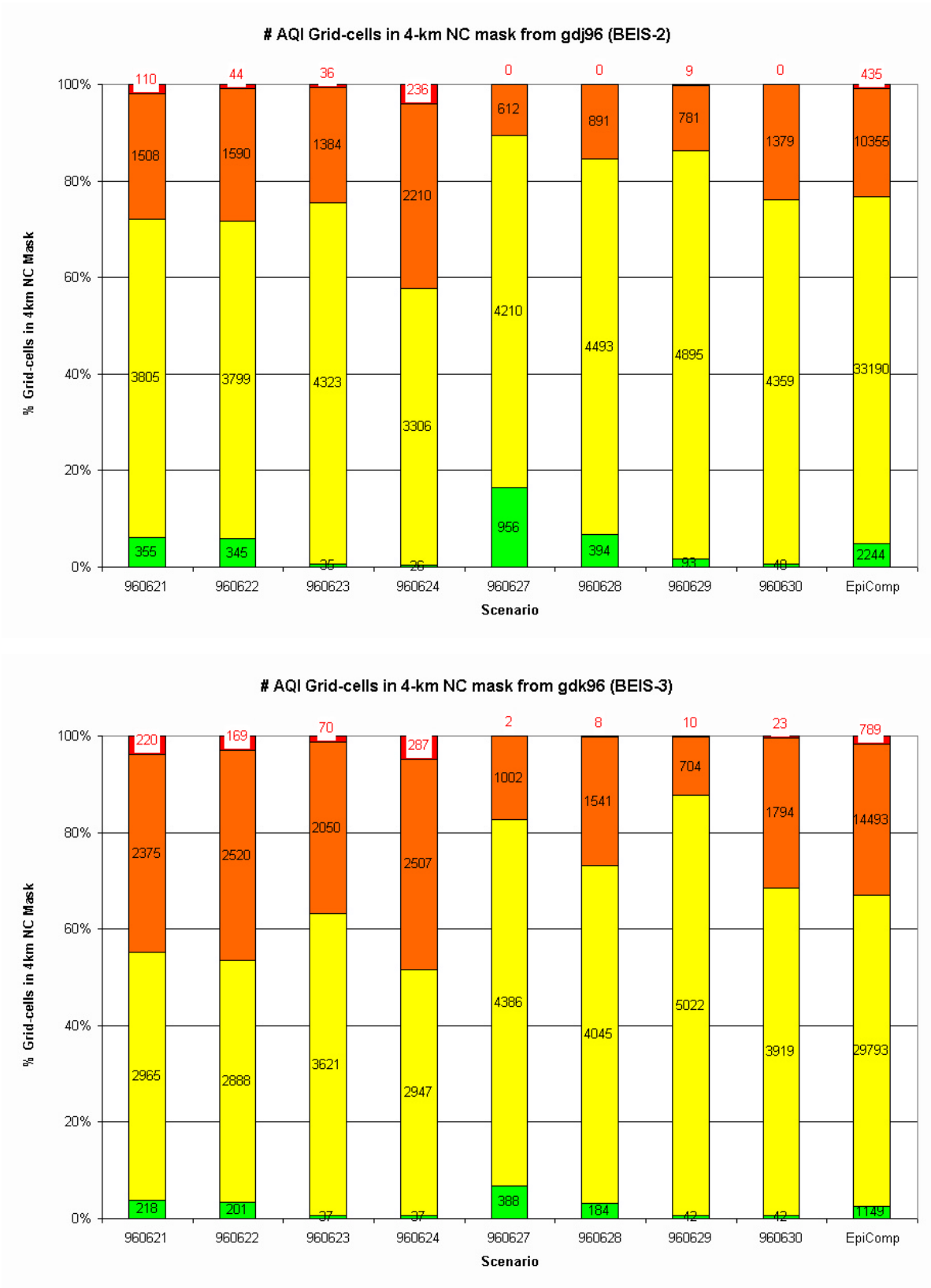
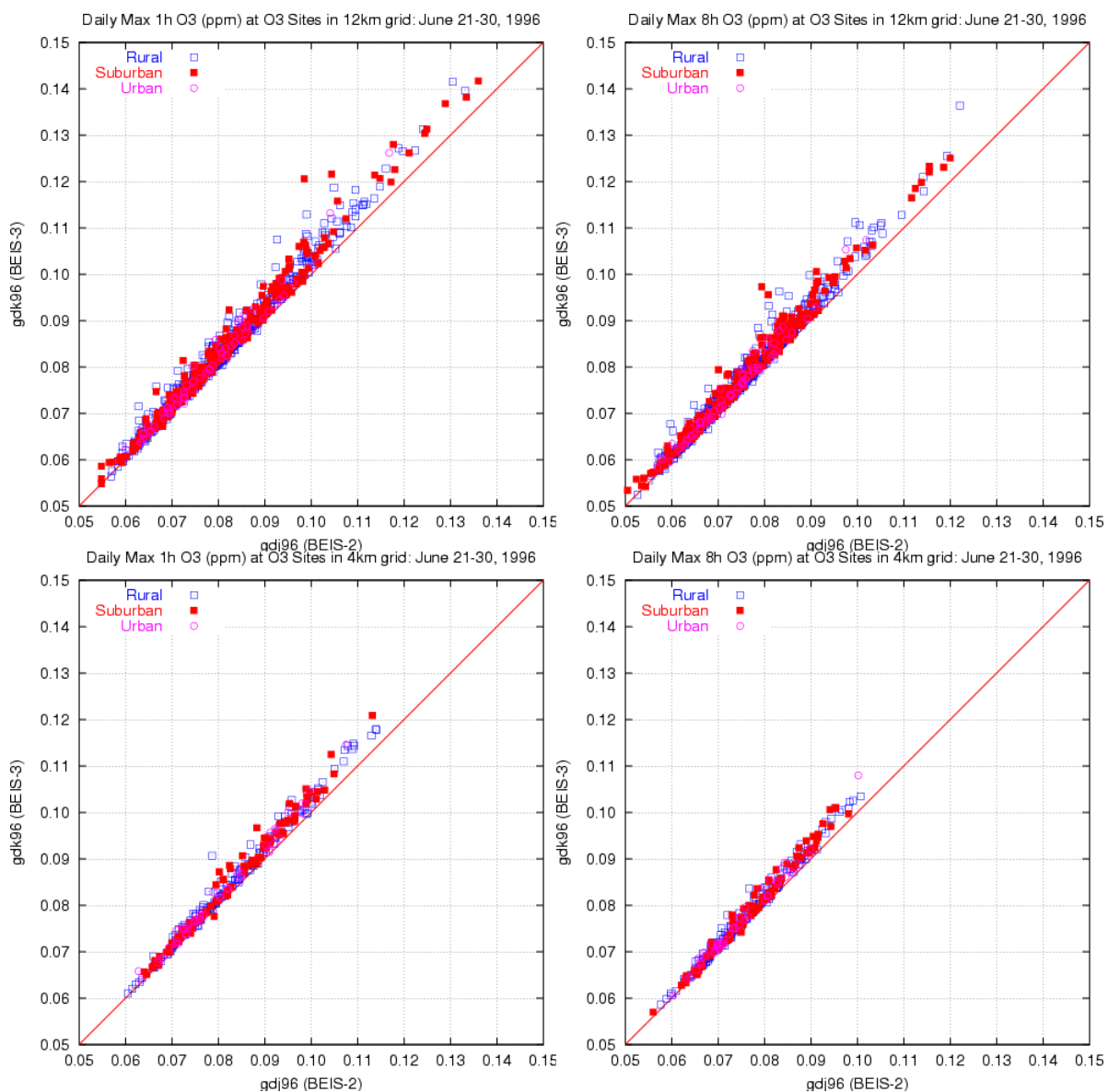


Figure 6. Scatter plots of daily maximum O₃ concentrations (ppm) in grid-cells containing O₃ monitors **a)** 1-h O₃ for sites in 12-km grid (top left), **b)** 8-h O₃ for sites in 12-km grid (top right), **c)** 1-h O₃ for sites in 4-km grid (bottom left), **d)** 8-h O₃ for sites in 4-km grid (bottom right).



CONCLUSIONS

We evaluated a prototype version of the new biogenic emissions inventory system, called BEIS-3 in MAQSIP modeling in a nested modeling domain in the Southeastern US. Explicit chemistry was added in MAQSIP's CB4 chemical mechanism to study the effects of large quantities of alcohol species (MEOH and ETOH) that were included in BEIS-3 estimates. We compared the model performance from two simulations (using BEIS-2 and BEIS-3) for 1-h and 8-h ozone at various thresholds, and overall the mean layer 1 ozone concentrations increased by 2-3 ppb on a domain-wide basis at all grid resolutions. This led to somewhat better model performance for 1-h ozone at a 60 ppb observed threshold. We also computed and compared various other metrics to assess the effect of revised estimates from BEIS-3. The increase in ozone predictions with BEIS-3 are somewhat expected since we added more ozone forming radicals (from the alcohol oxidation products) to the modeling system.

We are continuing to perform this evaluation, and have identified issues that need to be looked at for the future:

- Reconcile emissions estimates from BEIS-3/SMOKE with ambient data where available, especially for the newer alcohol species
- Use actual deposition velocities for MEOH and ETOH instead of the current PAR surrogates
 - o This might reveal if this process is an actual sink for these species
- Use IPR/IRR analyses to correlate formation of alcohol oxidation products with ozone
 - o We can identify differences in contribution to ozone from various processes/reactions, using the emissions estimates from BEIS-2 versus BEIS-3
- Evaluate model performance in upper layers
- Results from our ongoing work will be continuously updated and made available on MCNC's website.²⁸

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REFERENCES

1. US EPA. *Guideline for Regulatory Application of the Urban Airshed Model*, Office of Air Quality Planning and Standards, U.S. Environmental Protection Agency, Research Triangle Park, NC, 1991, EPA-450/4-91-013.
2. National Research Council (NRC), *Rethinking the Ozone Problem in Urban and Regional Air Pollution*, National Academic Press, Washington DC, 489 pp., 1991.
3. Lamb, B., D. Grosjean, B. Pun, and C. Seigneur, *Review of Emissions, Atmospheric Chemistry, and Gas/Particle Partition of Biogenic Volatile Organic Compounds and Reaction Products*, Document #CP051-1b-99, prepared for the Coordinating Research Council, Atmospheric and Environmental Research, Inc. CA, 1999.
4. Lamb, B., D. Gay, H. Westberg, and T. Pierce, A biogenic hydrocarbon emission inventory for the USA using a simple forest canopy model, *Atmos. Environ.* **1993**, 27A, 1673-1690.
5. Geron, C., A. Guenther, and T. Pierce, An improved model for estimating emissions of volatile organic compounds from forests in the eastern United States, *J. Geophys. Res.* **1994**, 99, 12773-12792.
6. Guenther, A., C.N. Hewitt, D. Erickson, R. Fall, C. Geron, T. Gradel, P. Harley, L. Klinger, M. Lerdau, T. Pierce, B. Scholes, R. Steinbrecher, R. Tallamraju, J. Taylor, and P. Zimmerman, A global model of natural volatile organic compound emissions, *J. Geophys. Res.* **1995**, 100, 8873-8892.
7. Guenther, A., C. Geron, T. Pierce, B. Lamb, P. Harley, and R. Fall, Natural emissions of non-methane volatile organic compounds, carbon monoxide, and oxides of nitrogen from North America, *Atmos. Environ.* **1999**, 34, 2205-2230.

8. NC Department of Environmental, Health and Natural Resources. *Protocol for Photochemical Air Quality Modeling of North Carolina*, prepared by Division of Air Quality and MCNC Environmental Programs, 1997.
9. Grell, G.A., J. Dudhia, and D.R. Stauffer. *A Description of the Fifth-Generation Penn State/NCAR Mesoscale Model (MM5)*, 1994, NCAR Technical Note TN-398, National Center for Atmospheric Research, Boulder, CO.
10. MM5 MCPL Meteorology Coupler. <http://www.emc.mcnc.org/projects/ppar/mcpl.html>, MCNC – Environmental Programs, RTP, NC. (Accessed Mar 2002)
11. Byun, D.W. and J.K.S. Ching, ed., *Science Algorithms of the EPA Models-3 Community Multiscale Air Quality (CMAQ) Modeling System*, 1999, EPA/600/R-99/030(peer reviewed). [Available from National Exposure Research Laboratory, Research Triangle Park, NC.
12. Dennis R.L., Byun D.W., Novak J.H., Galluppi K.J., Coats C.J. and Vouk M.A. The next generation of integrated air quality modeling: EPA's Models-3, *Atmos. Environ.* **1996**, 30, 1925-1938.
13. Kasibhatla, P. and W.L. Chameides, Seasonal modeling of regional O₃ pollution in the eastern U.S., *Geophys. Res. Lett.* **2000**, 27(9), 1415-1418.
14. Hogrefe, C., S.T. Rao, P. Kasibhatla, G. Kallos, C.J. Tremback, W. Hao, D. Olerud, A. Xiu, J. McHenry, and K. Alapaty, Evaluating the performance of regional-scale photochemical modeling systems: Part I – Meteorological predictions, submitted to *Atmos. Environ.* **2000**.
15. Hogrefe, C, S.T. Rao, P. Kasibhatla, W. Hao, G. Sistla, R. Mathur, and J. McHenry, Evaluating the performance of regional-scale photochemical modeling systems: Part II – Ozone predictions, submitted to *Atmos. Environ.* **2000**.
16. McHenry, J.N., N. Seaman, C. Coats, D. Stauffer, A. Gibbs, J. Vukovich, E. Hayes, N. Wheeler. The NCSC-PSU Numerical air quality prediction project: initial evaluation, status, and prospects, In *Proc. Symposium on Interdisciplinary Issues in Atmospheric Chemistry*, Amer. Meteor. Soc., Boston, MA, 95-102, 2000.
17. Odman, M. T., R. Mathur, A. F. Hanna, and D. W. Byun. Applications of the Multiscale Air Quality Simulation Platform (MAQSIP) to Regional Ozone Modeling. Presented at the *5th International Conference on Atmospheric Sciences & Applications to Air Quality*, June 18-20, 1996, Seattle, Washington, 1996.
18. Odman, M.T. and C. Ingram. Multiscale Air Quality Simulation Platform (MAQSIP), Source Code Documentation and Validation, MCNC Technical Report ENV-96TR002-v1.0, MCNC, Research Triangle Park, NC, 1996.
19. Gery, M.W., G.Z. Whitten, J.P. Killus, and M.C. Dodge. A photochemical kinetics mechanism for urban and regional scale computer modeling. *J. Geophys. Res.* **1989**, 94(D10), 12,925–12,956.
20. Houyoux, M., R. and J. M. Vukovich. Updates to the Sparse Matrix Operator Kernel Emissions (SMOKE) Modeling System and Integration with Models-3. In *Proceedings of The Emission Inventory: Regional Strategies for the Future, A&WMA Specialty Conference*, 26-28 October, Raleigh, NC, Air & Waste Management Association, 1999.
21. Vukovich, J. and T. Pierce, *The Implementation of BEIS-3 within the SMOKE modeling framework*, Presented at “Emissions Inventories – Partnering for the Future”, the 11th Emissions Inventory Conference of the U.S. Environmental Protection Agency, RTP, NC, 2002.
22. <ftp://ftp.epa.gov/amd/asmd/beld3/ascii> BELDv3.1 data
23. DeMore, W.B., S.P. Sander, D.M. Golden, R.F. Hampson, M.J. Kurylo, C.J. Howard, A.R. Ravishankara, C.E. Kolb, and M.J. Molina, *Chemical Kinetics and Photochemical Data for Use in Stratospheric Modeling*, Evaluation No. 12, JPL Publication# 97-4, Jet Propulsion Lab, California Institute of Technology, Pasadena, CA, 1997.
24. US EPA. *Draft Guidance on the Use of Models and other Analyses in attainment demonstrations for the 8-hour Ozone NAAQS*, Office of Air Quality Planning and Standards, U.S. Environmental Protection Agency, Research Triangle Park, NC, 1999, EPA-454/4-99-004.
25. Tesche T.W., Georgopoulos P., Seinfeld J.H., Cass G., Lurmann F.W., and Roth P.M. *Improvement of procedures for evaluating photochemical models*. Draft final report prepared for Research Division, California Air Resources Board, by Radian Corporation, Sacramento, CA, 1990.
26. Russell, A. and R. Dennis, NARSTO Critical Review of Photochemical Models and Modeling, *Atmos. Environ.* **2000**, 34, 2283-2324.
27. <http://www.epa.gov/airnow/aqibroch> (accessed Mar 2002).
28. <http://www.emc.mcnc.org/projects/NCDAQ/PGM/results/basecase96/gdk96/index.html> (accessed Mar 2002).

KEYWORDS

Ozone

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SIP

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